

=&gt; d que

L2 190 SEA FILE=REGISTRY ABB=ON PLU=ON (1042674-02-1/BI OR 1042674-31-6/BI OR 1042675-60-4/BI OR 10453-86-8/BI OR 106967-74-2/BI OR 1072-84-0/BI OR 115926-52-8/BI OR 122-04-3/BI OR 122-59-8/BI OR 129-46-4/BI OR 129318-43-0/BI OR 130-15-4/BI OR 13754-19-3/BI OR 145-73-3/BI OR 146903-18-6/BI OR 150560-58-0/BI OR 15084-51-2/BI OR 15516-47-9/BI OR 16037-91-5/BI OR 162086-14-8/BI OR 16629-19-9/BI OR 1710-98-1/BI OR 17325-26-7/BI OR 17630-76-1/BI OR 1821-12-1/BI OR 18496-54-3/BI OR 18711-13-2/BI OR 1878-49-5/BI OR 20142-87-4/BI OR 2058-74-4/BI OR 20780-76-1/BI OR 220965-34-4/BI OR 2243-83-6/BI OR 237756-11-5/BI OR 2632-13-5/BI OR 2650-44-4/BI OR 2687-25-4/BI OR 27318-90-7/BI OR 2905-27-3/BI OR 296771-71-6/BI OR 296773-88-1/BI OR 301166-54-1/BI OR 303092-45-7/BI OR 303149-87-3/BI OR 303998-01-8/BI OR 304883-18-9/BI OR 311321-81-0/BI OR 312519-17-8/BI OR 315671-49-9/BI OR 3282-30-2/BI OR 339205-70-8/BI OR 339205-73-1/BI OR 345630-40-2/BI OR 345630-42-4/BI OR 36043-49-9/BI OR 376383-76-5/BI OR 39755-95-8/BI OR 401646-54-6/BI OR 40926-73-6/BI OR 4122-68-3/BI OR 42494-71-3/BI OR 42494-73-5/BI OR 43100-25-0/BI OR 43100-38-5/BI OR 443-69-6/BI OR 452-58-4/BI OR 458553-48-5/BI OR 4755-77-5/BI OR 477847-81-7/BI OR 478063-72-8/BI OR 478077-73-5/BI OR 478077-74-6/BI OR 478077-78-0/BI OR 478077-79-1/BI OR 478257-55-5/BI OR 478257-73-7/BI OR 478257-76-0/BI OR 484-17-3/BI OR 496-72-0/BI OR 511518-73-3/BI OR 512796-41-7/BI OR 512796-49-5/BI OR 512796-50-8/BI OR 512796-65-5/BI OR 512796-67-7/BI OR 512796-72-4/BI OR 512796-76-8/BI OR 512796-99-5/BI OR 51630-58-1/BI OR 52315-07-8/BI OR 524-42-5/BI OR 5271-67-0/BI OR 52918-63-5/BI OR 5315-25-3/BI OR 5437-45-6/BI OR 547730-75-6/BI OR 5725-96-2/BI OR 585557-83-1/BI OR 586-75-4/BI OR 5908-27-0/BI OR 604-95-5/BI OR 610-14-0/BI OR 611-09-6/BI OR 619-05-6/BI OR 650620-84-1/BI

L7 59167 SEA FILE=REGISTRY ABB=ON PLU=ON 2404.11/RID

L8 512 SEA FILE=REGISTRY ABB=ON PLU=ON L7 AND 9,10-DIOXO?

L10 8 SEA FILE=REGISTRY ABB=ON PLU=ON L8 AND PHENOXY?

L11 2 SEA FILE=HCAPLUS ABB=ON PLU=ON L10

L12 32 SEA FILE=REGISTRY ABB=ON PLU=ON L2 AND L7

L18 1 SEA FILE=REGISTRY ABB=ON PLU=ON L2 AND C14 H9 N O2/MF

L19 1 SEA FILE=REGISTRY ABB=ON PLU=ON L2 AND C8 H6 CL2 O2/MF

L20 1 SEA FILE=REGISTRY ABB=ON PLU=ON L2 AND C9 H9 CL O2/MF

L21 1 SEA FILE=REGISTRY ABB=ON PLU=ON L2 AND C14 H7 N O4/MF

L23 59 SEA FILE=HCAPLUS ABB=ON PLU=ON L18 OR L21

L24 377 SEA FILE=HCAPLUS ABB=ON PLU=ON L19 OR L20

L25 1 SEA FILE=HCAPLUS ABB=ON PLU=ON L23 AND L24

L26 26 SEA FILE=REGISTRY ABB=ON PLU=ON L12 NOT S/ELS

L27 17 SEA FILE=REGISTRY ABB=ON PLU=ON L26 AND 4/NR

L28 5 SEA FILE=HCAPLUS ABB=ON PLU=ON L27

L29 5 SEA FILE=HCAPLUS ABB=ON PLU=ON L11 OR L28 OR L25

L30 5 SEA FILE=HCAPLUS ABB=ON PLU=ON L23 AND PHARM?/SC, SX

L31 8 SEA FILE=HCAPLUS ABB=ON PLU=ON L29 OR L30

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L31 ANSWER 1 OF 8 HCAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2008:1339565 HCAPLUS Full-text

DOCUMENT NUMBER: 149:509677  
 TITLE: Methods and compositions for stem cell self-renewal, particularly hematopoietic stem cell (HSC), by modulating PTEN and Wnt pathways  
 INVENTOR(S): Perry, John M.; Li, Linheng; Grindley, Justin C.  
 PATENT ASSIGNEE(S): Stowers Institute for Medical Research, USA  
 SOURCE: PCT Int. Appl., 110pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2008133904	A1	20081106	WO 2008-US5230	20080423
W: AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, NO, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
PRIORITY APPLN. INFO.:			US 2007-926065P	P 20070423
			US 2008-66693P	P 20080222

ED Entered STN: 07 Nov 2008

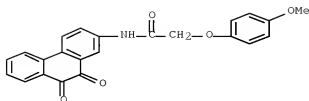
AB The present invention relates to methods for expanding a stem cell population without significant stem cell differentiation by modulating a PTEN phosphatase pathway and a Wnt pathway. More particularly, the invention relates, to methods and comps. for expanding a stem cell population, particularly a hematopoietic stem cell (HSC) population obtained from peripheral blood, cord blood, or bone marrow. The expanded HSC population comprises cells with a phenotype consisting of CD34-, CD34+/CD38-Thyl+/CD90+/Kit-/Lin-/CD133+/VEGFR2+, CD150+/CD48-/CD244-, CD150-/CD48-/CD244+, CD150-/CD48+/CD244+, and combinations thereof. In one embodiment the invention provides a kit for expanding HSC population for subsequent transplantation into a patient in need thereof. The kit comprises a PTEN inhibitor, a GSK-3 $\beta$  (glycogen synthase kinase 3 $\beta$ ) inhibitor, and instructions for the use of the inhibitors. It was demonstrated, that loss of PTEN with constitutively active  $\beta$ -catenin leads to HSC expansion with loss of early hematopoietic progenitors. It was also demonstrated, that ex vivo pharmacol. manipulation of the PTEN/Akt and Wnt/ $\beta$ -catenin signaling pathways cooperatively drive functional HSC expansion.

IT 867376-02-1, SF 1751

(reversible PTEN inhibitor; methods and comps. for stem cell self-renewal, particularly hematopoietic stem cell (HSC), by modulating PTEN and Wnt pathways)

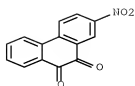
RN 867376-02-1 HCAPLUS

CN Acetamide, N-(9,10-dihydro-9,10-dioxo-2-phenanthrenyl)-2-(4-methoxyphenoxy)- (CA INDEX NAME)



CC 13-6 (Mammalian Biochemistry)  
 Section cross-reference(s): 3, 9, 63  
 IT 517-89-5, Shikonin 12179-38-3D, derivs. 367376-02-1, SF  
 1751  
 (reversible PTEN inhibitor; methods and compns. for stem cell  
 self-renewal, particularly hematopoietic stem cell (HSC), by  
 modulating PTEN and Wnt pathways)  
 REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR  
 THIS RECORD. ALL CITATIONS AVAILABLE IN THE  
 RE FORMAT

L31 ANSWER 2 OF 8 HCAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2008:1243425 HCAPLUS Full-text  
 DOCUMENT NUMBER: 149:524585  
 TITLE: Structure-Based Virtual Screening and Biological  
 Evaluation of Mycobacterium tuberculosis Adenosine  
 5'-Phosphosulfate Reductase Inhibitors  
 AUTHOR(S): Cosconati, Sandro; Hong, Jiyoung A.; Novellino,  
 Ettore; Carroll, Kate S.; Goodsell, David S.;  
 Olson, Arthur J.  
 CORPORATE SOURCE: Department of Molecular Biology, The Scripps  
 Research Institute, La Jolla, CA, 92037, USA  
 SOURCE: Journal of Medicinal Chemistry (2008), 51(21),  
 6627-6630  
 CODEN: JMCMAR; ISSN: 0022-2623  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 ED Entered STN: 16 Oct 2008  
 AB Tuberculosis is among the world's deadliest infectious diseases. APS  
 reductase catalyzes the first committed step in bacterial sulfate reduction  
 and is a validated drug target against latent tuberculosis infection. We  
 performed a virtual screening to identify APSR inhibitors. These inhibitors  
 represent the first non-phosphate-based mols. to inhibit APSR. Common  
 chemical features lay the foundation for the development of agents that could  
 shorten the duration of chemotherapy by targeting the latent stage of TB  
 infection.  
 IT 604-95-5  
 (structure-based screening and evaluation of M. tuberculosis APSR  
 inhibitors)  
 RN 604-95-5 HCAPLUS  
 CN 9,10-Phenanthrenedione, 2-nitro- (CA INDEX NAME)



CC 1-3 (Pharmacology)  
 IT 604-25-5 6942-44-5 13287-73-5 58160-29-5 113104-25-9  
 500576-09-0 501687-72-5 820999-41-5 873058-04-9 1073524-06-7  
 (structure-based screening and evaluation of M. tuberculosis APSR  
 inhibitors)  
 REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR  
 THIS RECORD. ALL CITATIONS AVAILABLE IN THE  
 RE FORMAT

L31 ANSWER 3 OF 8 HCAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2007:1167266 HCAPLUS Full-text  
 DOCUMENT NUMBER: 147:514411  
 TITLE: Planarity and Constraint of the Carbonyl Groups in  
 1,2-Diones Are Determinants for Selective  
 Inhibition of Human Carboxylesterase 1  
 AUTHOR(S): Hyatt, Janice L.; Wadkins, Randy M.; Tsurkan,  
 Lyudmila; Hicks, Latorya D.; Hatfield, M. Jason;  
 Edwards, Carol C.; Ross, Charles R., II;  
 Cantalupo, Stephanie A.; Crundwell, Guy; Danks,  
 Mary K.; Guy, R. Kip; Potter, Philip M.  
 CORPORATE SOURCE: Department of Molecular Pharmacology, St. Jude  
 Children's Research Hospital, Memphis, TN, 38105,  
 USA  
 SOURCE: Journal of Medicinal Chemistry (2007), 50(23),  
 5727-5734  
 CODEN: JMCMAR; ISSN: 0022-2623  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 147:514411  
 ED Entered STN: 17 Oct 2007

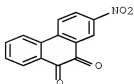
AB Carboxylesterases (CE) are ubiquitous enzymes responsible for the  
 detoxification of xenobiotics, including numerous clin. used drugs. Therefore,  
 the selective inhibition of these proteins may prove useful in modulating drug  
 half-life and bioavailability. Recently, we identified 1,2-diones as potent  
 inhibitors of CEs, although little selectivity was observed in the inhibition  
 of either human liver CE (hCE1) or human intestinal CE (hiCE). In this paper,  
 we have further examined the inhibitory properties of ethane-1,2-diones toward  
 these proteins and determined that, when the carbonyl oxygen atoms are cis-  
 coplanar, the compds. demonstrate specificity for hCE1. Conversely, when the  
 dione oxygen atoms are not planar (or are trans-coplanar), the compds. are  
 more potent at hiCE inhibition. These properties have been validated in over  
 40 1,2-diones that demonstrate inhibitory activity toward at least one of  
 these enzymes. Statistical anal. of the results confirms the correlation ( $P <$   
 0.001) between the dione dihedral angle and the preferential inhibition of  
 either hiCE or hCE1. Overall, the results presented here define the  
 parameters necessary for small mol. inhibition of human CEs.

IT 604-25-5  
 (Planarity and Constraint of the Carbonyl Groups in 1,2-Diones Are

## Determinants for Selective Inhibition of Human Carboxylesterase 1)

RN 604-95-5 HCAPLUS

CN 9,10-Phenanthrenedione, 2-nitro- (CA INDEX NAME)



CC 1-3 (Pharmacology)

Section cross-reference(s): 25, 27, 28

IT 82-86-0, Acenaphthoquinone 84-11-7, 9,10-Phenanthrenedione

134-81-6, Benzil 524-42-5, 1,2-Naphthoquinone 604-95-5

951-88-2, 1,2-Dicyclohexylethane-1,2-dione 1226-42-2 2103-62-0

2132-59-4 2767-84-2, (+/-)-Camphorquinone 3363-97-1 4290-72-6

4746-81-0, Mesitil 6067-45-4 6373-11-1, 1,2-Aceanthrylenedione

6706-92-9 16214-27-0, 1,2-Indandione 24243-31-0,

Benzo[1,2-b:4,3-b']dithiophene-4,5-dione 27471-02-9 40261-88-9

65938-98-9, Benzo[h]quinoline-5,6-dione

(Planarity and Constraint of the Carbonyl Groups in 1,2-Diones Are

Determinants for Selective Inhibition of Human Carboxylesterase 1)

REFERENCE COUNT: 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR  
THIS RECORD. ALL CITATIONS AVAILABLE IN THE  
RE FORMAT

L31 ANSWER 4 OF 8 HCAPLUS COPYRIGHT 2008 ACS ON STN

ACCESSION NUMBER: 2005:1123765 HCAPLUS Full-text

DOCUMENT NUMBER: 143:405906

TITLE: Preparation of (heteroaryl) amides and hydrazides  
as inhibitors of phosphatase located on chromosome  
10 (PTEN).

INVENTOR(S): Garlich, Joseph R.; Durden, Donald L.; Georgiadis,  
Taxiarchis M.; Su, Jingdong; Peng, Xiaodong;  
Smith, Tim C.

PATENT ASSIGNEE(S): Semafore Pharmaceuticals, Inc., USA

SOURCE: PCT Int. Appl., 85 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005097119	A2	20051020	WO 2005-US11626	20050406
WO 2005097119	A3	20060126		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA,  
CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI,  
GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM,  
KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN,  
MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC,  
SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG,  
US, UZ, VC, VN, YU, ZA, ZM, ZW

10/599,748

RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW,  
 AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ,  
 DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC,  
 NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA,  
 GN, GQ, GW, ML, MR, NE, SN, TD, TG

CA 2563316 A1 20051020 CA 2005-2563316 20050406  
 EP 1755574 A2 20070228 EP 2005-763900 20050406

R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU,  
 IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR

JP 2007532552 T 20071115 JP 2007-507462 20050406  
 US 20070203098 A1 20070830 US 2006-599748 20061006

PRIORITY APPLN. INFO.: US 2004-559802P P 20040406

US 2004-590043P P 20040720

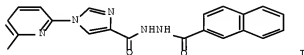
US 2004-625871P P 20041108

WO 2005-US11626 W 20050406

OTHER SOURCE(S): CASREACT 143:405906

ED Entered STN: 20 Oct 2005

GI



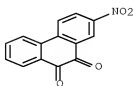
AB A method of protecting a patient from ≥1 treatments that trigger apoptosis comprises administration of a pharmaceutically acceptable amount of a PTEN inhibitor. Thus, 1-(6-methyl-2-pyridinyl)-1H-imidazole-4-carbohydrazide was stirred overnight with 2-naphthoyl chloride and Et3N in CH2Cl2 to give title compound (I). I gave 41-43% inhibition of PTEN at 250 μM.

IT 604-95-5P 36043-49-9P 345630-42-4P  
 860207-88-1P 867376-01-0P 867376-02-1P  
 867376-03-2P 867376-04-3P 867376-07-6P  
 867376-10-1P 867376-12-3P 867376-13-4P  
 867376-14-5P 867376-15-6P 867376-18-9P  
 867376-20-3P 867376-29-2P 867376-34-9P  
 867376-35-0P

(preparation of (heteroaryl) amides and hydrazides as inhibitors of phosphatase located on chromosome 10 (PTEN))

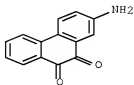
RN 604-95-5 HCAPLUS

CN 9,10-Phenanthredione, 2-nitro- (CA INDEX NAME)



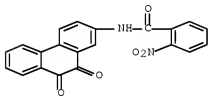
RN 36043-49-9 HCAPLUS

CN 9,10-Phenanthrenedione, 2-amino- (CA INDEX NAME)



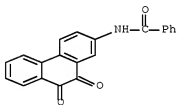
RN 345630-42-4 HCAPLUS

CN Benzamide, N-(9,10-dihydro-9,10-dioxo-2-phenanthrenyl)-2-nitro- (CA INDEX NAME)



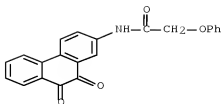
RN 860207-88-1 HCAPLUS

CN Benzamide, N-(9,10-dihydro-9,10-dioxo-2-phenanthrenyl)- (CA INDEX NAME)



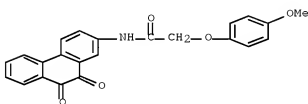
RN 867376-01-0 HCAPLUS

CN Acetamide, N-(9,10-dihydro-9,10-dioxo-2-phenanthrenyl)-2-phenoxy- (CA INDEX NAME)



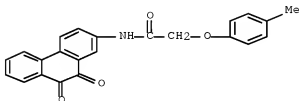
RN 867376-02-1 HCAPLUS

CN Acetamide, N-(9,10-dihydro-9,10-dioxo-2-phenanthrenyl)-2-(4-methoxyphenoxy)- (CA INDEX NAME)



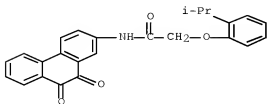
RN 867376-03-2 HCAPLUS

CN Acetamide, N-(9,10-dihydro-9,10-dioxo-2-phenanthrenyl)-2-(4-methylphenoxy)- (CA INDEX NAME)



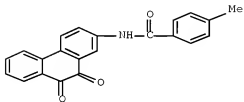
RN 867376-04-3 HCAPLUS

CN Acetamide, N-(9,10-dihydro-9,10-dioxo-2-phenanthrenyl)-2-[2-(1-methylethyl)phenoxy]- (CA INDEX NAME)



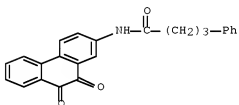
RN 867376-07-6 HCAPLUS

CN Benamide, N-(9,10-dihydro-9,10-dioxo-2-phenanthrenyl)-4-methyl- (CA INDEX NAME)



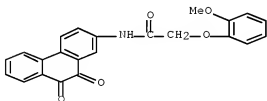
RN 867376-10-1 HCAPLUS

CN Benzenebutamide, N-(9,10-dihydro-9,10-dioxo-2-phenanthrenyl)- (CA INDEX NAME)



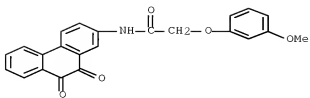
RN 867376-12-3 HCAPLUS

CN Acetamide, N-(9,10-dihydro-9,10-dioxo-2-phenanthrenyl)-2-(2-methoxyphenoxy)- (CA INDEX NAME)



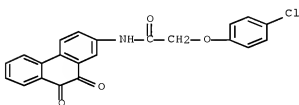
RN 867376-13-4 HCAPLUS

CN Acetamide, N-(9,10-dihydro-9,10-dioxo-2-phenanthrenyl)-2-(3-methoxyphenoxy)- (CA INDEX NAME)



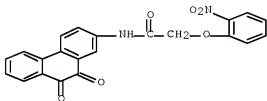
RN 867376-14-5 HCAPLUS

CN Acetamide, 2-(4-chlorophenoxy)-N-(9,10-dihydro-9,10-dioxo-2-phenanthrenyl)- (CA INDEX NAME)



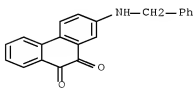
RN 867376-15-6 HCAPLUS

CN Acetamide, N-(9,10-dihydro-9,10-dioxo-2-phenanthrenyl)-2-(2-nitrophenoxy)- (CA INDEX NAME)



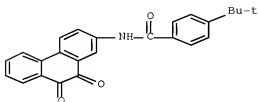
RN 867376-18-9 HCAPLUS

CN 9,10-Phenanthrenedione, 2-[(phenylmethyl)amino]- (CA INDEX NAME)



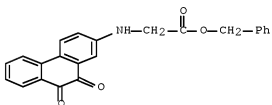
RN 867376-20-3 HCAPLUS

CN Benzamide, N-(9,10-dihydro-9,10-dioxo-2-phenanthrenyl)-4-(1,1-dimethylethyl)- (CA INDEX NAME)



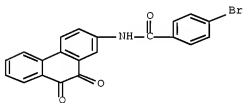
RN 867376-29-2 HCAPLUS

CN Glycine, N-(9,10-dihydro-9,10-dioxo-2-phenanthrenyl)-, phenylmethyl ester (CA INDEX NAME)



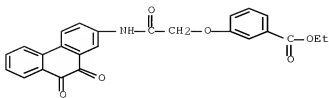
RN 867376-34-9 HCAPLUS

CN Benzamide, 4-bromo-N-(9,10-dihydro-9,10-dioxo-2-phenanthrenyl)- (CA INDEX NAME)

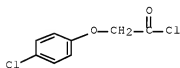


RN 867376-35-0 HCAPLUS

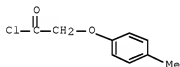
CN Benzoic acid, 3-[2-[(9,10-dihydro-9,10-dioxo-2-phenanthrenyl)amino]-2-oxoethoxy]-, ethyl ester (CA INDEX NAME)



IT 4122-68-3 15516-47-9  
 (preparation of (heteroaryl) amides and hydrazides as inhibitors of  
 phosphatase located on chromosome 10 (PTEN))  
 RN 4122-68-3 HCAPLUS  
 CN Acetyl chloride, 2-(4-chlorophenoxy)- (CA INDEX NAME)



RN 15516-47-9 HCAPLUS  
 CN Acetyl chloride, 2-(4-methylphenoxy)- (CA INDEX NAME)



IC ICM A61K031-44  
 CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))  
 Section cross-reference(s): 1  
 IT 504-95-5P 36043-49-5P 43100-25-0P 146903-18-6P  
 162086-14-8P 220965-34-4P 303092-45-7P 345630-40-2P  
 345630-42-4P 376383-76-5P 458553-48-5P 477847-81-7P  
 478257-76-0P 511518-73-3P 547730-75-6P 650620-84-1P  
 774184-51-9P 860207-88-1P 867339-05-7P 867375-71-1P  
 867375-74-4P 867375-77-7P 867375-78-8P 867375-79-9P  
 867375-82-4P 867375-88-0P 867375-89-1P 867375-90-4P  
 867375-91-5P 867375-92-6P 867375-93-7P 867375-94-8P  
 867375-96-0P 867375-97-1P 867375-99-3P 867376-00-9P  
 867376-01-0P 867376-02-1P 867376-03-2P  
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 867376-11-2P 867376-12-3P 867376-13-4P  
 867376-14-5P 867376-15-6P 867376-16-7P  
 867376-17-8P 867376-18-9P 867376-19-0P  
 867376-20-3P 867376-27-0P 867376-28-1P

867376-29-2P 867376-33-8P 867376-34-9P  
 867376-35-0P 867376-36-1P 867376-37-2P 867376-38-3P  
 867376-39-4P

(preparation of (heteroaryl) amides and hydrazides as inhibitors of phosphatase located on chromosome 10 (PTEN))

IT 79-04-9 95-54-5, 1,2-Benzenediamine, reactions 98-09-9,  
 Benzenesulfonyl chloride 98-59-9, Tosyl chloride 98-74-8,  
 4-Nitrobenzenesulfonyl chloride 122-04-3, 4-Nitrobenzoyl chloride  
 122-59-8 452-58-4, 2,3-Pyridinediamine 496-72-0 586-75-4  
 610-14-0 619-05-6 694-83-7, 1,2-Diaminocyclohexane 701-99-5,  
 Phenoxycetyl chloride 874-60-2 939-97-9, 4-tert-Butylbenzaldehyde  
 1072-84-0, 4-Imidazolecarboxylic acid 1710-98-1, 4-tert-Butylbenzoyl  
 chloride 1821-12-1, 4-Phenylbutyric acid 1878-49-5 2243-83-6,  
 2-Naphthoyl chloride 2687-25-4 2905-27-3 3282-30-2  
 4122-68-3 4755-77-5 5271-67-0, 2-Thiophenecarbonyl  
 chloride 5315-25-3, 2-Bromo-6-methylpyridine 5437-45-6  
 13754-19-3, 4,5-Pyrimidinediamine 15084-51-2,  
 4-tert-Butylbenzenesulfonyl chloride 15516-47-9  
 16629-19-9, 2-Thiophenesulfonyl chloride 17325-26-7, Methyl  
 imidazole-4-carboxylate 18496-54-3, 4-Phenylbutanoyl chloride  
 20142-87-4 40926-73-6 85397-21-3 106967-74-2 1042674-31-6  
 1042675-60-4

(preparation of (heteroaryl) amides and hydrazides as inhibitors of phosphatase located on chromosome 10 (PTEN))

L31 ANSWER 5 OF 8 HCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:472654 HCAPLUS Full-text

DOCUMENT NUMBER: 135:61559

TITLE: Preparation of phenanthrene-9,10-dione derivatives as CD45 inhibitors

INVENTOR(S): Chapdelaine, Marc Jerome; Knappenberger, Katherine; Steelman, Gary; Suchard, Suzanne; Sygowski, Linda; Urbanek, Rebecca; Veale, Chris Allan

PATENT ASSIGNEE(S): Astrazeneca AB, Swed.; Astrazeneca UK Limited  
 SOURCE: PCT Int. Appl., 42 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

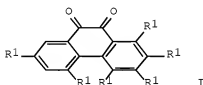
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001046125	A2	20010628	WO 2000-GB4854	20001218
WO 2001046125	A3	20020117		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
EP 1242363	A2	20020925	EP 2000-985603	20001218
EP 1242363	B1	20051102		
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR			
JP 2003518085	T	20030603	JP 2001-547036	20001218

10/599,748

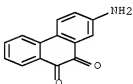
AT 308512	T	20051115	AT 2000-985603	20001218
US 20030207812	A1	20031106	US 2002-168758	20021125
PRIORITY APPLN. INFO.:			US 1999-172788P	P 19991221
			WO 2000-GB4854	W 20001218

OTHER SOURCE(S): MARPAT 135:61559  
 ED Entered STN: 29 Jun 2001  
 GI

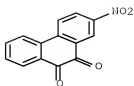


AB Substituted phenanthrene-9,10-diones I [R1 at each occurrence is independently selected from H, halogen, NH2, NO2, NHCOR2, CONHR2, Ar, (CH2)nCH(CO2H)R3, COR3, NHCOR2CH(CO2H)NHR4 and NR52, where R2 = (un)substituted (C1-C4)alkyl, (C1-C8)alkylCO2H or alkyl esters, Ph; n = 1-8; Ar = 3-thienyl, 2-benzofuranyl, 1-naphthyl, 1,3-benzodioxan-5-yl, or (un)substituted phenyl; R3 = certain N-linked oligopeptides; R4 = certain C-linked oligopeptides; R5 = H, tosyl (with provisos)] were prepared for the treatment of T cell mediated conditions such as autoimmune diseases and organ graft rejection. Thus, 9,10-dioxophenanthren-3-ylcarbonyl-Glu-Gln-Pro-Gln-Pro-OH was prepared by the solid-phase method and assayed for biol. activity (pNPP, lck, and T cell proliferation IC50s are 0.6, 2.4, and >30  $\mu$ M, resp. and CC50 is >30  $\mu$ M).

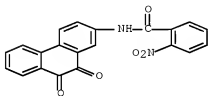
IT 36043-49-9P  
 (preparation of phenanthrenedione derivs. as CD45 inhibitors)  
 RN 36043-49-9 HCAPLUS  
 CN 9,10-Phenanthrenedione, 2-amino- (CA INDEX NAME)



IT 604-95-5P 345630-42-4P  
 (preparation of phenanthrenedione derivs. as CD45 inhibitors)  
 RN 604-95-5 HCAPLUS  
 CN 9,10-Phenanthrenedione, 2-nitro- (CA INDEX NAME)

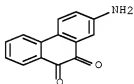


RN 345630-42-4 HCAPLUS  
 CN Benzamide, N-(9,10-dihydro-9,10-dioxo-2-phenanthrenyl)-2-nitro- (CA  
 INDEX NAME)

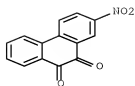


IC ICM C07C237-00  
 CC 34-3 (Amino Acids, Peptides, and Proteins)  
 Section cross-reference(s): 1, 15, 25  
 IT 604-94-4P 32060-67-6P 32155-34-3P 36043-49-9P  
 47194-23-0P 49546-41-0P 51789-39-0P 53622-33-6P 109497-01-0P  
 345631-37-0P 345631-41-6P 345631-42-7P  
 (preparation of phenanthrenedione derivs. as CD45 inhibitors)  
 IT 604-94-4P 4733-06-6P 7473-71-4P 13292-03-0P  
 62896-78-0P 109313-55-5P 345630-35-5P 345630-37-7P  
 345630-38-8P 345630-40-2P 345630-42-4P 345630-43-5P  
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 345631-38-1P 345631-39-2P 345631-40-5P 345631-43-8P  
 345631-44-9P  
 (preparation of phenanthrenedione derivs. as CD45 inhibitors)

L31 ANSWER 6 OF 8 HCAPLUS COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 2001:306240 HCAPLUS [Full-text](#)  
 DOCUMENT NUMBER: 135:70647  
 TITLE: Potent Reversible Inhibitors of the Protein  
 Tyrosine Phosphatase CD45  
 AUTHOR(S): Urbanek, Rebecca A.; Suchard, Suzanne J.;  
 Steelman, Gary B.; Knappenberger, Katharine S.;  
 Sygowski, Linda A.; Veale, Chris A.; Chapdelaine,  
 Marc J.  
 CORPORATE SOURCE: AstraZeneca Pharmaceuticals, Wilmington, DE,  
 19850, USA  
 SOURCE: Journal of Medicinal Chemistry (2001), 44(11),  
 1777-1793  
 PUBLISHER: CODEN: JMCNAR; ISSN: 0022-2623  
 DOCUMENT TYPE: American Chemical Society  
 LANGUAGE: Journal  
 English  
 ED Entered STN: 02 May 2001  
 AB The cytosolic portion of CD45, a major transmembrane glycoprotein found on  
 nucleated hematopoietic cells, contains protein tyrosine phosphatase activity  
 and is critical for T-cell receptor-mediated T-cell activation. CD45  
 inhibitors could have utility in the treatment of autoimmune disorders and  
 organ graft rejection. A number of 9,10-phenanthrenediones were identified  
 that reversibly inhibited CD45-mediated p-nitrophenyl phosphate (pNPP)  
 hydrolysis. Chemical efforts around the 9,10-phenanthrenedione core led to  
 the most potent inhibitors known to date. In a functional assay, the compds.  
 were also potent inhibitors of T-cell receptor-mediated proliferation, with  
 activities in the low micromolar range paralleling their enzyme inhibition.  
 It was also discovered that the nature of modification to the  
 phenanthrenedione pharmacophore could affect selectivity for CD45 over PTP1B  
 (protein tyrosine phosphatase 1B) or vice versa.  
 IT 36043-49-9P  
 (preparation and structure activity relationships of phenanthrenediones  
 as inhibitors of protein tyrosine phosphatase CD45)  
 RN 36043-49-9 HCAPLUS  
 CN 9,10-Phenanthrenedione, 2-amino- (CA INDEX NAME)



IT 604-95-5P  
 (preparation and structure activity relationships of phenanthrenediones  
 as inhibitors of protein tyrosine phosphatase CD45)  
 RN 604-95-5 HCAPLUS  
 CN 9,10-Phenanthrenedione, 2-nitro- (CA INDEX NAME)



CC 1-3 (Pharmacology)

Section cross-reference(s): 25

IT 604-94-4P 32155-34-3P 36043-49-9P 53622-33-6P

345631-41-6P

(preparation and structure activity relationships of phenanthrenediones as inhibitors of protein tyrosine phosphatase CD45)

IT 604-95-5P 607-09-0P 13292-03-0P 32060-67-6P

47194-23-0P 51789-39-0P 62896-78-0P 73671-07-5P 109497-01-0P

137354-59-7P 345224-95-5P 345224-96-6P 345224-97-7P

345224-98-8P 345224-99-9P 345630-35-5P 345630-37-7P

345630-38-8P 345630-40-2P 345630-43-5P 345630-46-8P

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345631-39-2P 345631-42-7P 345631-43-8P 345631-44-9P

346717-82-6P 346717-83-7P

(preparation and structure activity relationships of phenanthrenediones as inhibitors of protein tyrosine phosphatase CD45)

REFERENCE COUNT: 66 THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L31 ANSWER 7 OF 8 HCAPLUS COPYRIGHT 2008 ACS ON STN

ACCESSION NUMBER: 1922:15423 HCAPLUS Full-text

DOCUMENT NUMBER: 16:15423

ORIGINAL REFERENCE NO.: 16:2684h-i, 2685a-i

TITLE: Amino- and anilinophenanthrenequinones

AUTHOR(S): Brass, Kurt; Ferber, Erwin

SOURCE: Berichte der Deutschen Chemischen Gesellschaft

[Abteilung] B: Abhandlungen (1922), 55B, 541-56

CODEN: BDCBAD; ISSN: 0365-9488

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

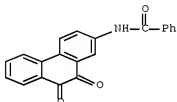
ED Entered STN: 16 Dec 2001

AB cf. C. A. 14, 3070. 2-Bromophenanthrenequinone (A), treated with PhNH<sub>2</sub>, PhNH<sub>2</sub>.HCl or 2PhNH<sub>2</sub>.H<sub>2</sub>SO<sub>4</sub> under ordinary conditions, under pressure or in PhNO<sub>2</sub> as a diluent, does not react with elimination of HBr, but the A acts as an oxidizing agent and the resulting dark blue to black products are substances closely related to aniline black. If they are freed from the

excess of PhNH<sub>2</sub> and the unchanged A is removed with alkaline Na<sub>2</sub>S<sub>2</sub>O<sub>4</sub>, they can easily be oxidized to benzoquinone with CrO<sub>3</sub>; the 2-bromophenanthrenequinol (B) formed simultaneously, however, also reacts with any PhNH<sub>2</sub> still present with the formation of phenylaminohydroxyphenanthrene. The same results are obtained when AcNHPh or its Na salt or the Na or Al salts of PhNH<sub>2</sub> are used instead of PhNH<sub>2</sub>. The monophenylhydrazone of A does not react with PhNH<sub>2</sub> in the desired sense, nor does the dibenzoate of B. Recourse was then had to the phenylation of aminophenanthrenequinones. 2- and 4-Nitrophenanthrenequinones are obtained in 20 and 13 g. yields, resp., by nitration of 30 g. phenanthrenequinone. The 2-NO<sub>2</sub> compound (5 g.), rubbed to a thin paste with 250 cc. NaOH (d. 1.065), slowly treated with somewhat more than 4 mols. solid Na<sub>2</sub>S<sub>2</sub>O<sub>4</sub>, warmed a short time at 50°, diluted, filtered and treated with air, gives 3.6 g. of the 2-NH<sub>2</sub> compound (C), also obtained in 3.9 g. yield from 5 g. of the NO<sub>2</sub> compound in much H<sub>2</sub>O quickly treated with a solution of NaSH prepared from 1.6 g. NaOH, shaken 0.5 hr. in a tightly stoppered flask, diluted and treated with air; it seps. from H<sub>2</sub>O in slender black-violet needles, brown in transmitted light, sinters 205-10°, gradually softens but does not m. clear 300°, soluble in concentrated H<sub>2</sub>SO<sub>4</sub> with red-brown, in H<sub>2</sub>SO<sub>4</sub> diluted with 0.25 part H<sub>2</sub>O with cress-red, in fuming acid (20% SO<sub>3</sub>) with green color; acetyl derivative (D), obtained with Ac<sub>2</sub>O in boiling AcOH, red-violet needles from the red-brown solution in PhNO<sub>2</sub>, m. 324° (decomposition), soluble in concentrated H<sub>2</sub>SO<sub>4</sub> with brown, in H<sub>2</sub>SO<sub>4</sub>-H<sub>2</sub>O (4 : 1) with red-brown, in fuming acid with green color, easily forms a yellow vat from which it is reprecipitated (passing through green) by air, dyes cotton a dirty salmon-red; benzoyl derivative, prepared with BzCl in hot C<sub>5</sub>H<sub>5</sub>N, flat brown-red spears from PhNO<sub>2</sub>, m. 297-8°, soluble in H<sub>2</sub>SO<sub>4</sub> with green-brown color, forms a deep-yellow vat which dyes cotton a turbid light red. 2-Acetylamino-o,o'-diacetylphenanthrenequinol, from C in a little AcOH heated a short time with excess of Ac<sub>2</sub>O and then boiled about 0.5 hr. with Fe filings, fine white needles from EtOH-H<sub>2</sub>O, m. 228°, subliming in silky needles, gradually dissolves in concentrated H<sub>2</sub>SO<sub>4</sub> with green color. 4-Aminophenanthrenequinone, obtained almost quantitatively from the NO<sub>2</sub> compound with NaSH and subsequent treatment with air, violet-brown crystalline meal with metallic luster from H<sub>2</sub>O, black warty aggregates from 96% alc., softens 207°, does not m. 340°, easily soluble in the usual solvents with intense red, in concentrated H<sub>2</sub>SO<sub>4</sub> with yellow-olive, in more dilute acid (4 : 1) with red-brown color. 2-Ethylaminophenanthrenequinone, from 1.7 g. D and 0.9 g. EtBr heated 5.5 hrs. at 180° in C<sub>5</sub>H<sub>5</sub>N in a sealed tube, poured into much dilute HCl, filtered and deacetylated by boiling 1.5 hrs. with 1 : 1 H<sub>3</sub>PO<sub>4</sub>, violet-black powder, soluble in hot AcOH, PhNO<sub>2</sub> and C<sub>5</sub>H<sub>5</sub>N with brown color, seps. from PhNO<sub>2</sub> in crystalline warts, has no m. p. 2-Anilinophenanthrenequinone, from equimol. ams. of C and PhBr, with a little Cu powder, heated 4 hrs. at 200° in C<sub>5</sub>H<sub>5</sub>N, black, almost insol. powder, soluble in cold concentrated H<sub>2</sub>SO<sub>4</sub> with dirty brown color, forms a vat with very great difficulty in aqueous, easily in aqueous alc. suspension, has no m. p., is almost insol. in aqueous or alc. KOH. 2',4'-Dinitro-2-anilinophenanthrenequinone, obtained (together with some [(O<sub>2</sub>N)C<sub>2</sub>H<sub>3</sub>-]₂, m. 143°) from 1 mol. each of C and 2,4-(O<sub>2</sub>N)C<sub>2</sub>H<sub>3</sub>Cl, with a little CaCO<sub>3</sub> and Cu powder boiled 1.5 hrs. in PhNO<sub>2</sub>, brown spear- and table-like crystals from PhNO<sub>2</sub>, m. 280°, soluble in concentrated H<sub>2</sub>SO<sub>4</sub> with brown color, forms a vat in alkaline Na<sub>2</sub>S<sub>2</sub>O<sub>4</sub>, does not react with o-C<sub>6</sub>H<sub>4</sub>(NH<sub>2</sub>)<sub>2</sub>, forms in cold aqueous alc. KOH a salt recognized by the intense red color imparted to the solution, gives 2,4-(O<sub>2</sub>N)C<sub>2</sub>H<sub>3</sub>OH with K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub>-H<sub>2</sub>SO<sub>4</sub> (no diphenic acid could be detected); 1 g. heated 1 hr. at 80° with 100 cc. of 10% KOH gives 2',4'-dinitro-2-anilindiphenylethyleneglycolic acid, brown amorphous powder, has no m. p., soluble in concentrated H<sub>2</sub>SO<sub>4</sub> with red-brown color, forms easily soluble alkali and insol. Pb, Cu and Ag salts. 2',4',6'-Trinitro-2-anilinophenanthrenequinone, from C and 1 mol. picryl chloride, with a little NaOAc and a trace of Cu powder, refluxed 3 hrs. in alc., sandy powder of small red-brown table-like crystals or a red to red-brown amorphous powder, m. 304-5°, soluble in concentrated H<sub>2</sub>SO<sub>4</sub> with yellow-green color, reprecipitated. unchanged

by H<sub>2</sub>O, forms a vat with alkaline Na<sub>2</sub>S<sub>2</sub>O<sub>4</sub> but gives no quinoxaline with o-C<sub>6</sub>H<sub>4</sub>(NH<sub>2</sub>)<sub>2</sub>, oxidized by K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub>-H<sub>2</sub>SO<sub>4</sub> to picramide, gives with aqueous KOH 2',4',6'-trinitro-2-anilindiphenyleneglycolic acid, does not m., decomp. 300° (heated in larger amts. in an open test-tube it deflagrates explosively at 160°).

IT 860207-88-1P, Benzamide,  
N-(9,10-dihydro-9,10-diketo-2-phenanthryl)-  
(preparation of)  
RN 860207-88-1 HCAPLUS  
CN Benzamide, N-(9,10-dihydro-9,10-dioxo-2-phenanthrenyl)- (CA INDEX  
NAME)



CC 10 (Organic Chemistry)  
IT 4733-06-6P, Acetamide, N-(9,10-dihydro-9,10-diketo-2-phenanthryl)-  
4733-06-6P, Phenanthrenequinone, 2-acetamido- 109497-01-0P,  
Phenanthrenequinone, 4-amino- 860207-88-1P, Benzamide,  
N-(9,10-dihydro-9,10-diketo-2-phenanthryl)- 860207-88-1P,  
Phenanthrenequinone, 2-benzamido- 861321-00-8P, 9-Fluorene-carboxylic  
acid, 9-hydroxy-2-(2,4,6-trinitroanilino)- 861337-30-6P,  
Phenanthrenequinone, 2-anilino- 861349-60-2P, Phenanthrenequinone,  
2-(2,4,6-trinitroanilino)- 861349-63-5P, Phenanthrenequinone,  
2-ethylamino- 861350-08-5P, Acetamide,  
N-(9,10-dihydroxy-2-phenanthryl)-, diacetate 861350-08-5P,  
9,10-Phenanthrenediol, 2-acetamido-, diacetate 861373-57-1P,  
9-Fluorene-carboxylic acid, 2-(2,4-dinitroanilino)-9-hydroxy-  
861798-82-5P, Phenanthrenequinone, 2-(2,4-dinitroanilino)-  
(preparation of)

L31 ANSWER 8 OF 8 HCAPLUS COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 1916:14053 HCAPLUS Full-text  
DOCUMENT NUMBER: 10:14053  
ORIGINAL REFERENCE NO.: 10:2583a-i,2584a-c  
TITLE: Dyes derived from phenanthraquinone  
AUTHOR(S): Mukherjee, Kshitish C.; Watson, Edwin R.  
CORPORATE SOURCE: Dacca, Bengal, India  
SOURCE: Journal of the Chemical Society, Transactions  
(1916), 109, 617-28  
CODEN: JCHTA3; ISSN: 0368-1645  
DOCUMENT TYPE: Journal  
LANGUAGE: Unavailable

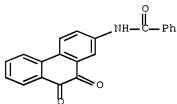
ED Entered STN: 16 Dec 2001

AB A study undertaken because of the close relationship of phenanthraquinone (A) to anthraquinone (B). The methods of introducing additional HO groups used in the (B) series failed, owing to the feeble resistance of the (A) series, but the methods used for the production of anilino derivs. (Ullmann, Ber. 34, 2174(1901), and D. R. P. 113,011) were applicable. Attempts to obtain vat dyes from acylamino derivs. were not encouraging. 15 g. fuming H<sub>2</sub>SO<sub>4</sub> (SO<sub>3</sub> =

70%) were added to 1.5 g. 2-hydroxyphenanthraquinone in a small stoppered bottle which was kept closed at 35-40° for 48 hrs.; the resulting acid was isolated as barium 2-hydroxyphenanthraquinonesulfonate, violet, soluble in boiling H<sub>2</sub>O, insol. in absolute alc. 3 g. 2,7-diacetoxypheanthraquinone in 30 cc. HNO<sub>3</sub> (d. 1.39) were warmed to 50-60° for 1.5 min. by immersion in boiling H<sub>2</sub>O, followed by immediately pouring into H<sub>2</sub>O, giving nitro-2,7-diacetoxypheanthraquinone, yellow-brown prisms, does not m. 290°; boiled in HOAc containing a few drops H<sub>2</sub>SO<sub>4</sub> it yields nitro-2,7-dihydroxyphenanthraquinone (C), brown, does not m. below 290°. (C), heated on the H<sub>2</sub>O bath with Sn and concentrated HCl, did not dissolve, but turned first deep brown and then light brown; then warmed first with aqueous FeCl<sub>3</sub> solution and boiled with dilute HCl until ash-free it gave amino-2,7-dihydroxyphenanthraquinone, plates, does not m. 290°, insol. in organic solvents, soluble in alkalis with a brown color; triacetyl derivative, amorphous; diazotization and boiling gave 2,4(?),7-trihydroxyphenanthraquinone, red-brown, does not m. 290°, soluble in alkalis with a brown color; triacetate, red-brown microcrystals, m. about 280°. 2,7-Diaminophenanthraquinone, NaOAc, and Ac<sub>2</sub>O heated at 160° for 1 hr., mixed with an equal volume of HOAc, and poured into H<sub>2</sub>O, gave the diacetamino derivative, chocolate-brown crystals, does not m. below 295°. 1 g. dibromophenanthraquinone (D), from (A) in PhNO<sub>2</sub> with Br (D. R. P. 222,206), when boiled with 35 cc. HNO<sub>3</sub> (d. 1.42) for 0.5 hr. and the solution poured into H<sub>2</sub>O, gave dibromonitrophenanthraquinone, yellow needles, m. 244-5°; 1 g. (D), boiled 2 min. with 10 cc. fuming HNO<sub>3</sub> (d. 1.51) and 1.5 cc. H<sub>2</sub>SO<sub>4</sub> and poured into H<sub>2</sub>O gave bromodinitrophenanthraquinone, yellow needles, m. above 300°. 2-Nitrophenanthraquinone (1 g.), 0.6 g. Br, and 6 cc. HOAc at 140° for 2 hrs. gave bromo-2-nitrophenanthraquinone (E), red-yellow plates, m. above 300°. 1 g. 4-nitrophenanthraquinone treated with excess of Br at 110° in as little PhNO<sub>2</sub> as possible gave the bromo derivative, yellow prisms, m. 224-6°; 1 g. 2,7-dibromophenanthraquinone, 10 g. PhNH<sub>2</sub>, and 0.25 g. Cu powder were boiled for 2.5-3 hrs., filtered hot, and poured into an excess of dilute HCl; the resulting blue-black 2,7-dianilinophenanthraquinone does not m. below 300° and dyes wool blue-black shades. Similarly (D) gives a bluish dianilinophenanthraquinone, does not m. below 300° and dyes wool greenish blue shades; (E) yielded 2-nitroanilinophenanthraquinone (F), blue-black, does not m. below 300°, dyes wool blue-black shades; 4-nitroanilinophenanthraquinone, black, does not m. below 300°, dyes wool blackish shades; dinitroanilingphenanthraquinone, black, gives greenish black shades on wool; nitrodianilinophenanthraquinone, dyes wool in black shades. Dianilinophenanthraquinone, heated with 10 parts H<sub>2</sub>SO<sub>4</sub> (d. 1.84) at 110-20° for 1 hr. gives a sulfonic acid which dyes faster, greener shades than the parent substance. Similarly, at 125-30° for 2 hrs. (F) gives a sulfonic acid which dyes chrome-mordanted wool in olive-green shades. 1 g. (D), 1 g. p-O<sub>2</sub>N<sub>2</sub>C<sub>6</sub>H<sub>4</sub>NH<sub>2</sub>, 5 cc. PhNMe<sub>2</sub>, and a trace of Cu powder heated at 160° for 3.5 hrs. and poured into dilute HCl gave bromo-p-nitroanilinophenanthraquinone, reddish violet, does not m. 280°, does not dye wool. 1 g. (D), 1.5 g. (C<sub>6</sub>H<sub>4</sub>NH<sub>2</sub>)<sub>2</sub>, 2 g. fused NaOAc, 0.35 g. CuCl<sub>2</sub>, and 20 g. PhNO<sub>2</sub> boiled for 2 hrs., precipitated with Et<sub>2</sub>O, washed with alc., and boiled with H<sub>2</sub>O gave dibenzidindiphenanthraquinone, black powder, does not m., does not dye wool. 2-Aminophenanthraquinone and BzCl in PhNO<sub>2</sub> at 100° for 20 min. gave the benzoyl derivative, pinkish needles, m. 295°; as a vat dye it gives pale pink shades on cotton; 2-phthalylaminophenanthraquinone, pale orange needles, does not m. 295°, dyes cotton pale yellow in the vat; 2-oxalylaminophenanthraquinone, red-brown needles, does not m. 295°, does not dye cotton. 2,7-Dibenzoyldiaminophenanthraquinone, using BzCl in boiling PhNO<sub>2</sub>, brick-red needles, does not m. 295°, in the vat gives brown-orange shades on cotton; 2,7-diphthalylldiaminophenanthraquinone, brick-red needles, does not m. 295°, is not absorbed from the vat by cotton; 2,7-diaminophenanthraquinonesulfonic acid, using excess of fuming acid (SO<sub>3</sub> = 70%) in a closed bottle for 48 hrs.

and pouring into H<sub>2</sub>O; in the moist state it dyes alummordanted wool dull green shades. Phenanthraquinonebisazophenol, diazotizing in 5% H<sub>2</sub>SO<sub>4</sub> suspension, adding to a PhOH solution, and carefully making alkaline with Na<sub>2</sub>CO<sub>3</sub>, lenticular crystals, does not m. 295°, soluble in alkalis with a brown color; boiling with Ac<sub>2</sub>O and a drop of C<sub>5</sub>H<sub>5</sub>N and precipitating with alc. gives the acetate, brick-red prisms, m. 274°.

IT 860207-88-1P, Phenanthrenequinone, 2-benzamido-  
(preparation of)  
RN 860207-88-1 HCAPLUS  
CN Benzamide, N-(9,10-dihydro-9,10-dioxo-2-phenanthrenyl)- (CA INDEX NAME)



CC 10 (Organic Chemistry)  
IT 49546-41-0P, Phenanthrenequinone, 2,7-diamino-, diaceto derivative  
860207-88-1P, Phenanthrenequinone, 2-benzamido-  
860208-68-0P, Phenanthrenequinone, 2,4,7-trihydroxy-, triaceto derivative  
860208-68-0P, Phenanthrenequinone, 2,4,7-trihydroxy- 860208-69-1P,  
Phenanthrenequinone, 2-(phthalylamino)- 860208-70-4P,  
Phenanthrenequinone, 2,7-dibenzamido- 860768-28-1P,  
Phenanthrenequinone, 2,7-bis(phthalylamino)- 860768-29-2P,  
Phenanthrenequinone, anilino-4-nitro- 871902-28-2P,  
Phenanthrenequinone, 2,7-dianilino-  
(preparation of)

=> d his nofile

(FILE 'HOME' ENTERED AT 08:44:52 ON 17 DEC 2008)

FILE 'HCAPLUS' ENTERED AT 08:45:03 ON 17 DEC 2008

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SEL RN

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L3 1 SEA ABB=ON PLU=ON L2 AND C22 H15 N O4/MF

FILE 'HCAPLUS' ENTERED AT 08:48:30 ON 17 DEC 2008

L4 1 SEA ABB=ON PLU=ON L3

FILE 'REGISTRY' ENTERED AT 08:48:57 ON 17 DEC 2008

E C22 H15 N O4/MF

L5 409 SEA ABB=ON PLU=ON "C22 H15 N O4"/MF  
L6 39 SEA ABB=ON PLU=ON L5 AND 10-DIOXO?  
L7 59167 SEA ABB=ON PLU=ON 2404.11/RID  
L8 512 SEA ABB=ON PLU=ON L7 AND 9,10-DIOXO?  
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L10 8 SEA ABB=ON PLU=ON L8 AND PHENOXY?

FILE 'HCAPLUS' ENTERED AT 08:52:45 ON 17 DEC 2008

L11 2 SEA ABB=ON PLU=ON L10

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L15      0 SEA ABB=ON PLU=ON L12 AND BENZOXY?
L16      0 SEA ABB=ON PLU=ON L12 AND BENZYLOXY?
L17      0 SEA ABB=ON PLU=ON L8 AND BENZYLOXY?
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L19      1 SEA ABB=ON PLU=ON L2 AND C8 H6 CL2 O2/MF
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L24      377 SEA ABB=ON PLU=ON L19 OR L20
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L26      26 SEA ABB=ON PLU=ON L12 NOT S/ELS
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FILE 'HCAPLUS' ENTERED AT 09:08:20 ON 17 DEC 2008
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L29      5 SEA ABB=ON PLU=ON L11 OR L28 OR L25
L30      5 SEA ABB=ON PLU=ON L23 AND PHARM7/SC,SX
L31      8 SEA ABB=ON PLU=ON L29 OR

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